Molecular-Level Modeling of Metal and Ceramic Cutting and Grinding

Computer simulations used to improve fabrication methods for precision components

We are developing molecular-level computer models of the cutting and grinding processes used to fabricate high-precision components. The simulations are specifically aimed at understanding the precision cutting of silicon optics (such as for gas laser systems) and, more generally, at understanding cutting-tool wear. Processes such as single-point diamond turning of metal surfaces and ductile grinding of glass surfaces can be used to fabricate components with a dimensional tolerance (or a surface finish) of only a few tens of nanometers. However, little is understood at the atomic level of the mechanisms that determine how material is removed and deformed, and how the tool tip (or the individual abrasives used in the grinding process) interacts with the workpiece and causes wear. Computer simulations allow us to visualize these processes and predict surface and subsurface damage.

APPLICATIONS

- *Develop more accurate, reliable machining methods*
- *Develop surface-finishing processes that eliminate cracking and increase strength*
- *Develop more cost-efficient processes for manufacturing ceramic components*

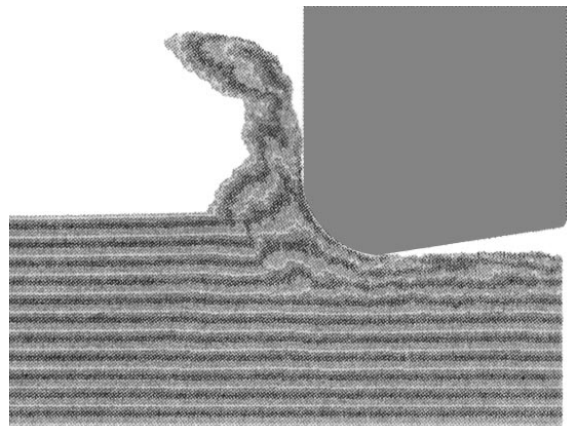
Computer simulations

We have developed several simulation programs for use on massively parallel computers to predict large-scale deformation at the atomic level. The simplest approach, called molecular dynamics (MD) simulation, calculates the motion of every atom in a material as it is being machined.

The accompanying snapshot is from our steady-state MD simulation of orthogonal metal cutting. The shaded bands, which represent layers of atoms, enhance the visualization to show the motion of the dislocations made by the cutting process.

An example application

One industrial application for our computer simulations is to improve the fabrication of ceramic components for new automotive and truck engines. Engines made with ceramic components can operate at higher temperatures and thus will be more efficient. However, ceramics are notoriously sensitive to brittle fracture and are expensive to fabricate to the dimensional tolerances needed for engines while maintaining low damage and high strength. With MD modeling, we can develop a surface-finishing process that minimizes cracking and increases the strength of the ceramics so they can be used economically in the next generation of engines.



Snapshot from a steady-state MD simulation of orthogonal metal cutting. Calculated cutting forces agree remarkably well with experimental measurements.

Availability: The technology is available now. We are looking for industrial collaborators to continue the development of molecular modeling codes.

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